What is claimed is:

1. A method for identifying a polypeptide that binds a ligand, comprising:

(a) comparing a sequence of a polypeptide
5 to a sequence model for polypeptides that bind a ligand, wherein said sequence model comprises representations of amino acids consisting of a subset of amino acids, said subset of amino acids having one or more atom within a selected distance from a bound ligand in said
10 polypeptides that bind said ligand; and

(b) determining a relationship between said sequence and said sequence model, wherein a correspondence between said sequence and said sequence model identifies said polypeptide as a polypeptide that
15 binds said ligand.

2. The method of claim 1, wherein said sequence model comprises a nucleic acid sequence.

3. The method of claim 1, wherein said sequence model comprises an amino acid sequence.

20   4. The method of claim 1, wherein one of said sequence models is a Hidden Markov Model.

5. The method of claim 1, wherein one of said sequence models is a Support Vector Machines Model.

6. The method of claim 1, wherein one of said sequence models is a Position Specific Score Matrices Model.

7. The method of claim 1, wherein one of said
5 sequence models is a Neural Network Model.

8. The method of claim 1, further comprising the step of:

(c) producing a sequence model with a set of sequences, said set of sequences consisting of
10 sequences of polypeptides having a subset of amino acids, said subset of amino acids having one or more atom within a selected distance from a bound ligand in said polypeptides that bind said ligand.

9. The method of claim 8, further comprising
15 the steps of:

(d) adding a sequence of said identified polypeptide that binds said ligand to said set of sequences; and

(e) repeating steps (a) through (c) one or
20 more times.

10. The method of claim 1, wherein said sequence model is produced by the steps of:

(a) identifying a subset of amino acids having one or more atom within a selected distance from a bound conformation of a ligand in a set of polypeptides that bind said ligand; and

(b) producing a sequence model, amino acids of said sequence model consisting of said subset of amino acids.

11. A method for identifying a member of a pharmacofamily, comprising:

(a) comparing a sequence of a polypeptide to a sequence model for polypeptides of a pharmacofamily; and

(b) determining a relationship between said sequence and said sequence model, wherein a correspondence between said sequence and said sequence model identifies said polypeptide as a member of said pharmacofamily.

12. The method of claim 11, wherein said sequence model comprises a nucleic acid sequence.

13. The method of claim 11, wherein said sequence model comprises an amino acid sequence.

14. The method of claim 11, wherein said sequence model is a Hidden Markov Model.

15. The method of claim 11, wherein said sequence model is a Support Vector Machines Model.

16. The method of claim 11, wherein said sequence model is a Position Specific Score Matrices Model.

17. The method of claim 11, wherein one of said sequence models is a Neural Network Model.

18. The method of claim 11, further comprising the step of:

(c) producing a sequence model with a set of sequences, said set of sequences consisting of sequences of polypeptides in said pharmacofamily.

19. The method of claim 18, further comprising the steps of:

(d) adding a sequence of said identified member of said pharmacofamily to said set of sequences; and

(e) repeating steps (a) through (c) one or more times.

20. The method of claim 11, wherein said sequence model comprises representations of amino acids consisting of a subset of amino acids, said subset of amino acids having one or more atom within a selected distance from a bound ligand in said polypeptides of said pharmacofamily.

21. The method of claim 20, wherein said sequence model is produced by the steps of:

(a) identifying a subset of amino acids in a pharmacofamily having one or more atom within a selected distance from a bound conformation of a ligand; and

(b) producing a sequence model, amino acids of said sequence model consisting of said subset of amino acids.

22. A method for identifying a member of a pharmacofamily, comprising:

(a) comparing a sequence of a polypeptide to a sequence model and a differential sequence model; and

(b) determining a relationship between said sequence and said sequence models, wherein a correspondence between said sequence and said sequence models identifies said polypeptide as a member of said pharmacofamily.

23. The method of claim 22, wherein said sequence model comprises a nucleic acid sequence.

24. The method of claim 22, wherein said sequence model comprises an amino acid sequence.

25. The method of claim 22, wherein one of said sequence models is a Hidden Markov Model.

26.   The method of claim 22, wherein one of said sequence models is a Support Vector Machines Model.

27.   The method of claim 22, wherein one of said sequence models is a Position Specific Score

5 Matrices Model.

28.   The method of claim 22, wherein one of said sequence models is a Neural Network Model.

29.   The method of claim 22, further comprising the step of:

10   (c) producing a sequence model with a set of sequences, said set of sequences consisting of sequences of polypeptides in said pharmacofamily.

30.   The method of claim 29, further comprising the steps of:

15   (d) adding a sequence of said identified member of said pharmacofamily to said set of sequences; and

        (e) repeating steps (a) through (c) one or more times.

20   31.   The method of claim 22, wherein said differential sequence model comprises representations of amino acids consisting of a subset of amino acids, said subset of amino acids having one or more atom within a selected distance from a bound ligand in said

25 polypeptides of said pharmacofamily.

32. The method of claim 31, wherein said differential sequence model is produced by the steps of:

(a) identifying a subset of amino acids in a pharmacofamily having one or more atom within a
5 selected distance from a bound conformation of a ligand; and

(b) producing a differential sequence model, amino acids of said differential sequence model consisting of said subset of amino acids.

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